A COMBINED EXPERIMENTAL AND THEORETICAL APPROACH TO INTERFACE STRUCTURE AND PROPERTIES*

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Z-contrast scanning transmission electron microscopy combined with electron energy loss spectroscopy provides an essentially complete atomic-scale characterization of interfaces. Atomic structure and impurity segregation sites can be determined directly from experiment. Such data is a perfect starting point for first-principles theoretical calculations, providing total energies, diffusion pathways, activation barriers, and the link to properties. For As in Si, images show segregation in particular atomic columns in a grain boundary, and calculations show the As to be in the form of dimers. In MgO, an impurity-induced structural transformation has been revealed, while in $SrTiO_3$, a grain boundary reconstruction is observed, and spontaneous creation of vacancies predicted by theory. At the Si/SiO_2 interface, the structure of the last crystalline plane is seen directly in the image, and composition profiles show a significant zone of sub-stoichiometric oxide. Theory, however, shows abrupt interfaces are energetically preferred. *Z*-contrast images of single-walled carbon nanotubes show iodine inside the tubes in a double helix configuration. Theory confirms this as a low energy configuration, and shows how doping occurs by charge transfer.

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*This research was sponsored by the Division of Materials Sciences, U. S. Department of Energy under contract No. DE-AC05-96OR22464 with Lockheed Martin Energy Research Corp.